

Full wwPDB X-ray Structure Validation Report (i)

Oct 25, 2023 – 09:27 PM EDT

PDB ID	:	3BH7
Title	:	Crystal structure of the RP2-Arl3 complex bound to GDP-AlF4
Authors	:	Veltel, S.; Gasper, R.; Wittinghofer, A.
Deposited on		
Resolution	:	1.90 Å(reported)
1		1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

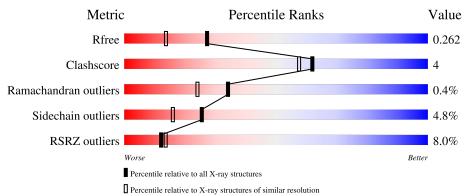
Xtriage (Phenix) EDS buster-report Percentile statistics	: : :	20191225.v01 (using entries in the PDB archive December 25th 2019)
-	:	
CCP4 Ideal geometry (proteins)		7.0.044 (Gargrove) Engh & Huber (2001)
Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP)		

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain	
1	А	164	9%	14% •
2	В	352	80%	8% • 11%



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 4016 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

• Molecule 1 is a protein called ADP-ribosylation factor-like protein 3.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	А	161	Total 1296	C 823	N 221	0 248	${S \atop 4}$	0	3	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	14	GLY	-	expression tag	UNP Q9WUL7
А	15	GLY	-	expression tag	UNP Q9WUL7
А	16	SER	-	expression tag	UNP Q9WUL7

• Molecule 2 is a protein called Protein XRP2.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
2	В	314	Total 2467	C 1569	N 408	0 471	S 19	0	1	0

There are 2 discrepancies between the modelled and reference sequences:

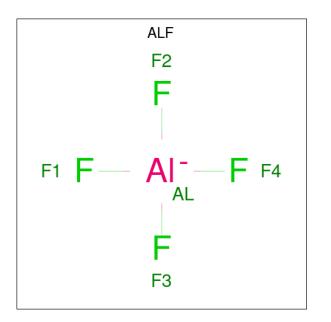
Chain	Residue	Modelled	Actual	Comment	Reference
В	-1	GLY	-	expression tag	UNP 075695
В	0	SER	-	expression tag	UNP 075695

• Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total Mg 1 1	0	0

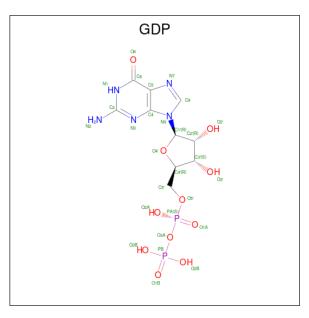
• Molecule 4 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF₄).





Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
4	A	1	Total 5	Al 1	F 4	0	0

• Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
5	А	1	Total 28	C 10	N 5	0 11	Р 2	0	0

• Molecule 6 is water.

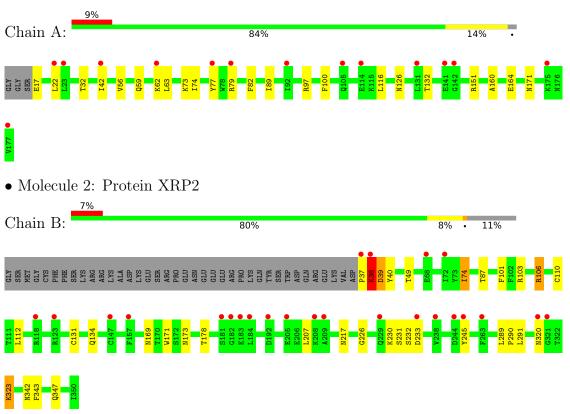


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	65	$\begin{array}{cc} \text{Total} & \text{O} \\ 65 & 65 \end{array}$	0	0
6	В	154	Total O 154 154	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.



• Molecule 1: ADP-ribosylation factor-like protein 3



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	73.70Å 77.94Å 97.92Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.73 - 1.90	Depositor
Resolution (A)	19.60 - 1.90	EDS
% Data completeness	$100.0\ (19.73-1.90)$	Depositor
(in resolution range)	98.8 (19.60-1.90)	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	0.04	Depositor
$< I/\sigma(I) > 1$	$4.03 (at 1.90 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
D D.	0.232 , 0.262	Depositor
R, R_{free}	0.230 , 0.262	DCC
R_{free} test set	2228 reflections (5.00%)	wwPDB-VP
Wilson B-factor $(Å^2)$	28.9	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.42, 53.8	EDS
L-test for twinning ²	$ < L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4016	wwPDB-VP
Average B, all atoms $(Å^2)$	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.93% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, ALF, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain Bor		nd lengths	Bond angles	
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.37	0/1327	0.55	0/1796
2	В	0.54	1/2518~(0.0%)	0.54	0/3408
All	All	0.49	1/3845~(0.0%)	0.54	0/5204

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	В	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(Å)	Ideal(Å)
2	В	226	GLY	C-O	-5.00	1.15	1.23

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	В	38	LYS	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	1296	0	1305	15	0
2	В	2467	0	2415	19	0
3	А	1	0	0	0	0
4	А	5	0	0	0	0
5	А	28	0	12	0	0
6	А	65	0	0	1	0
6	В	154	0	0	2	0
All	All	4016	0	3732	33	0

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (33) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:B:110:CYS:HB3	6:B:478:HOH:O	1.72	0.88
2:B:37:PRO:O	2:B:38:LYS:HD3	1.81	0.80
1:A:126:ASN:HD21	1:A:160:ALA:H	1.29	0.77
2:B:291:LEU:HD11	2:B:323:LYS:HG3	1.72	0.72
2:B:37:PRO:O	2:B:38:LYS:CB	2.44	0.65
2:B:37:PRO:O	2:B:38:LYS:CG	2.46	0.64
2:B:37:PRO:O	2:B:38:LYS:CD	2.46	0.63
1:A:59:GLN:HE22	1:A:171:ASN:HA	1.70	0.57
1:A:116:LEU:O	1:A:151:ARG:NH2	2.38	0.56
2:B:38:LYS:HA	2:B:40:TYR:H	1.72	0.55
2:B:38:LYS:C	2:B:40:TYR:H	2.10	0.55
2:B:37:PRO:O	2:B:38:LYS:HB3	2.07	0.54
2:B:134:GLN:HG3	2:B:173:ASN:O	2.09	0.52
2:B:169:ASN:HD21	2:B:171:TRP:HB3	1.75	0.52
1:A:56:VAL:HG23	1:A:63:LEU:HB2	1.90	0.52
1:A:59:GLN:NE2	1:A:171:ASN:OD1	2.44	0.51
1:A:74:ILE:HG22	1:A:77[B]:TYR:CE2	2.45	0.51
1:A:17:GLU:HB3	6:A:230:HOH:O	2.12	0.49
2:B:87:THR:HG23	2:B:106:ARG:HG3	1.95	0.49
1:A:74:ILE:HG22	1:A:77[B]:TYR:HE2	1.78	0.49
1:A:73:LYS:HD3	2:B:178:THR:HG22	1.96	0.48
1:A:97:ARG:HG2	1:A:100:PHE:CE2	2.50	0.47
2:B:38:LYS:CA	2:B:40:TYR:H	2.27	0.47
1:A:79:ARG:HG3	1:A:82:PHE:CE2	2.49	0.47
1:A:22:LEU:HD12	1:A:89:ILE:HB	1.96	0.46

Continued on next page...



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:112:LEU:HD23	6:B:478:HOH:O	2.14	0.46
1:A:97:ARG:NH1	1:A:132:THR:O	2.49	0.45
2:B:74:ILE:O	2:B:74:ILE:HG12	2.16	0.45
1:A:32:THR:O	1:A:42:ILE:HD11	2.17	0.44
2:B:289:LEU:N	2:B:290:PRO:HD2	2.33	0.44
2:B:131:CYS:H	2:B:169:ASN:ND2	2.17	0.43
2:B:38:LYS:C	2:B:40:TYR:N	2.74	0.40

Continued from previous page...

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	А	162/164~(99%)	159~(98%)	3~(2%)	0	100	100
2	В	312/352~(89%)	309~(99%)	1 (0%)	2(1%)	25	15
All	All	474/516~(92%)	468 (99%)	4 (1%)	2~(0%)	34	24

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	В	38	LYS
2	В	39	ASP

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	144/142~(101%)	141 (98%)	3~(2%)	53 48
2	В	276/311 (89%)	258 (94%)	18 (6%)	17 8
All	All	420/453~(93%)	399~(95%)	21 (5%)	25 15

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	62[A]	LYS
1	А	62[B]	LYS
1	А	164	GLU
2	В	39	ASP
2	В	49	THR
2	В	74	ILE
2	В	101	PHE
2	В	103	ARG
2	В	106	ARG
2	В	207	LEU
2	В	217	ASN
2	В	230	LYS
2	В	231	SER
2	В	232	SER
2	В	233	ASP
2	В	245	TYR
2	В	320	ASN
2	В	323	LYS
2	В	342	ASN
2	В	343	PHE
2	В	347	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	59	GLN
1	А	64	ASN
1	А	126	ASN
1	А	154	GLN
1	А	171	ASN
1	А	176	ASN
2	В	61	GLN
2	В	88	ASN
2	В	149	GLN

Continued on next page...



Continued from previous page...

	•	-	- 0
Mol	Chain	\mathbf{Res}	Type
2	В	158	GLN
2	В	169	ASN
2	В	175	HIS
2	В	196	GLN
2	В	217	ASN
2	В	303	ASN
2	В	320	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol Type Ch		Chain	Dec	Dog	Dog	Bos	Dec	Dec	Dog	Dec	Res Link		Bond lengths			Bond angles		
IVIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2								
5	GDP	А	2	3	24,30,30	1.01	1 (4%)	30,47,47	1.08	3 (10%)								
4	ALF	А	3	-	0,4,4	-	-	-										

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.



'-' means no outliers of that kind were identified.

N	Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
	5	GDP	А	2	3	-	2/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(Å)	Ideal(Å)
5	А	2	GDP	C6-N1	-2.50	1.34	1.37

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
5	А	2	GDP	C8-N7-C5	2.57	107.89	102.99
5	А	2	GDP	C5-C6-N1	2.32	118.05	113.95
5	А	2	GDP	O2B-PB-O3A	2.27	112.24	104.64

There are no chirality outliers.

All (2) torsion outliers are listed below:

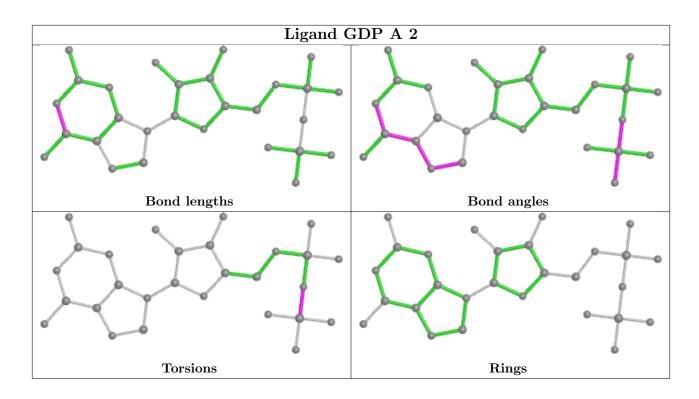
Mol	Chain	Res	Type	Atoms
5	А	2	GDP	PA-O3A-PB-O2B
5	А	2	GDP	PA-O3A-PB-O1B

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ $>$	#RSRZ>2		$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	Q < 0.9
1	А	161/164~(98%)	0.63	14 (8%) 10 1	11	18, 29, 38, 41	0
2	В	314/352~(89%)	0.69	24 (7%) 13 1	15	15, 29, 41, 53	1 (0%)
All	All	475/516~(92%)	0.67	38 (8%) 12 1	13	15, 29, 40, 53	1 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	В	245	TYR	7.0
1	А	131	LEU	5.5
2	В	38	LYS	5.0
2	В	157	PHE	4.8
2	В	320	ASN	4.7
2	В	37	PRO	4.1
2	В	233	ASP	3.7
2	В	244	ASP	3.2
2	В	181	SER	3.2
1	А	114	GLU	3.2
2	В	192	ASP	3.2
1	А	141	GLU	3.1
1	А	62[A]	LYS	3.1
2	В	321	GLY	3.0
2	В	209	ALA	3.0
2	В	183	GLU	2.8
1	А	105	GLN	2.8
2	В	205	GLU	2.7
1	А	77[A]	TYR	2.7
2	В	72	ILE	2.7
1	А	92	ILE	2.6
2	В	238	VAL	2.6
2	В	184	LEU	2.5
1	А	23	LEU	2.5

Continued on next page...



Mol	Chain	Res	Type	RSRZ
1	А	79	ARG	2.5
1	А	175	LYS	2.5
2	В	263	PHE	2.5
2	В	182	GLY	2.4
2	В	229	GLN	2.3
1	А	142	GLY	2.3
2	В	208	LYS	2.2
1	А	22	LEU	2.2
2	В	68	GLU	2.2
1	А	177	VAL	2.2
2	В	147	CYS	2.1
1	А	42	ILE	2.1
2	В	118[A]	ARG	2.0
2	В	123	ARG	2.0

Continued from previous page...

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

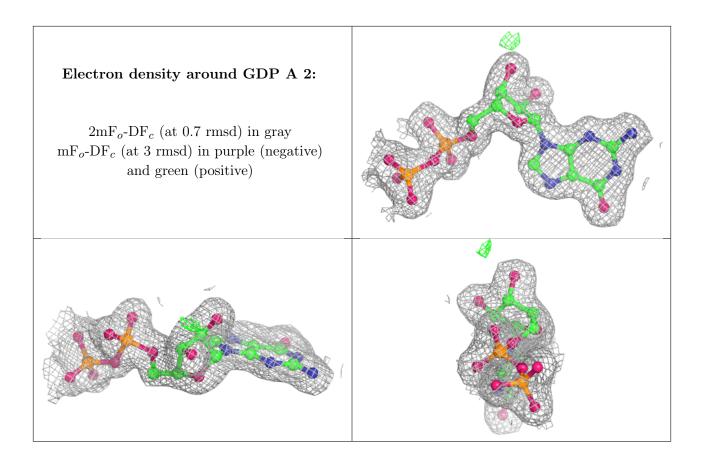
6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q < 0.9
4	ALF	А	3	5/5	0.98	0.07	$21,\!22,\!23,\!23$	0
5	GDP	А	2	28/28	0.98	0.10	17,22,23,23	0
3	MG	А	1	1/1	0.99	0.08	18,18,18,18	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers (i)

There are no such residues in this entry.

